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MEMORANDUM FOR PRR (~~Contractor~~/In-House Publication)

2 June1999

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Jeff Mills, "Hydrocarbon Fuels Optimization"

Poster Session – HEDM Conference

(Public Release)

Hydrocarbon Fuels Optimization

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Introduction–

Hydrocarbon fuels, as a class, are investigated using the minimal set of parameters determinative of oxidizer-optimized specific impulse and common density-specific-impulse analogues. In this context specific families of promising candidate fuels can be systematically compared, the performance trade-offs among the relevant chemical and physical properties can be quantified, and the general characteristics of mission-tailored fuels can begin to be elucidated.

Initial Questions–

?

- Why do I sometimes get relatively poor theoretical performance from a high-energy hydrocarbon?
- Why is RP-1 (kerosene) such a good rocket fuel?
- What are the minimal set of fuel parameters that determine hydrocarbon I_{sp}?
- What are the performance trade-offs among these parameters?
- How can I begin to use this information to search for the "optimum" hydrocarbon fuel and reduce "hunt and peck" methods?

General Concepts/Initial Approximations–

Characteristics of “Good” Rocket Fuels:

- High Heat of Formation
- High “Light-Atom” Content

Specific Impulse:

(Momentum Transfer from Combusted Ejecta)

For an optimal nozzle:

$$I_{sp} \equiv \frac{1}{g}\sqrt{2\left(H_{chamb.} - H_{exh.}\right)}$$

Sometimes approximated:

$$(I_{sp})_{opt} \propto \frac{1}{g}\sqrt{2\,\Delta H_{comb.}}$$

or,

$$(I_{sp})_{opt} \propto \frac{1}{g}\sqrt{2\,\Delta H_f}$$

ΔH_{comb}–stoichiometric combustion enthalpy (per unit mass of exhaust products)

ΔH_f–specific enthalpy of formation

More Realistic Model Rocket–

One-Dimensional, Adiabatic, Equilibrated, Isentropic Expansion from the Combustion Chamber

Reference Rocket Conditions for I_{sp} Optimized vs. LOX:

Sea level expansion:

$$P_{chamber} = 1000\,\text{psi},\ P_{exhaust} = 14.7\,\text{psi}$$

"Vacuum" expansion:

$$P_{chamber} = 1000\,\text{psi},\ \epsilon = 40$$

Sole determinative parameters of LOX-optimized specific impulse and its density variants:

$$(I_{sp})_{opt} \Leftarrow \Delta H_f(/g) \text{ and } r(\tfrac{H}{C})$$

$$(\rho_{of}^{a}\, I_{sp})_{opt} \Leftarrow \Delta H_f(/g),\ r(\tfrac{H}{C}),\ \rho_f,\ \text{and } a$$

$\Delta H_f(/g)$–specific enthalpy of formation of the fuel

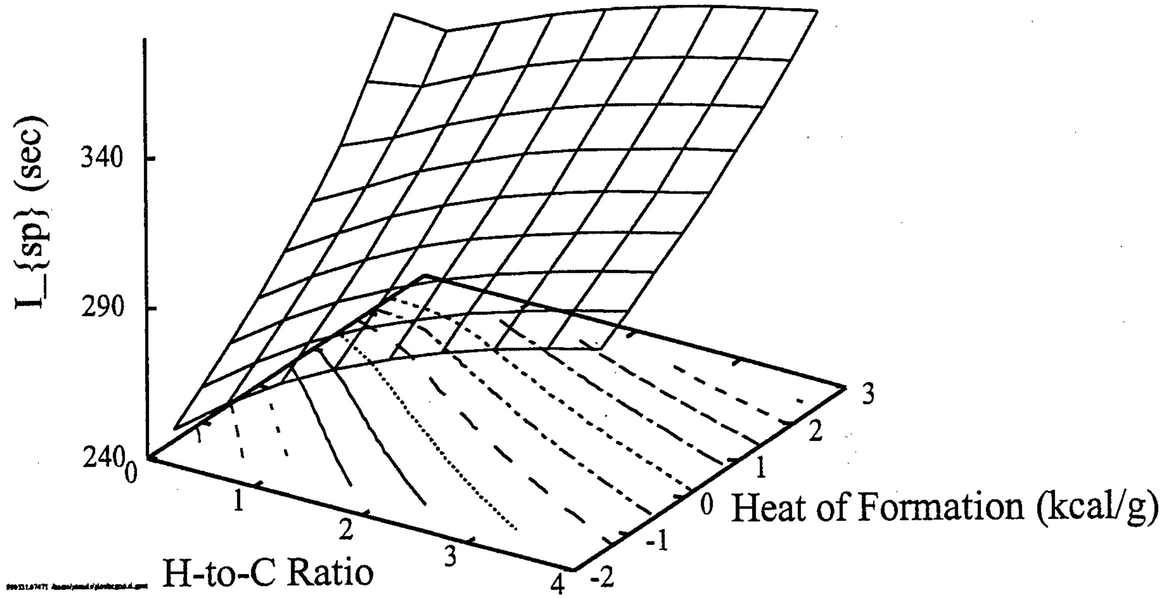
$r(\frac{H}{C})$–atom ratio of fuel

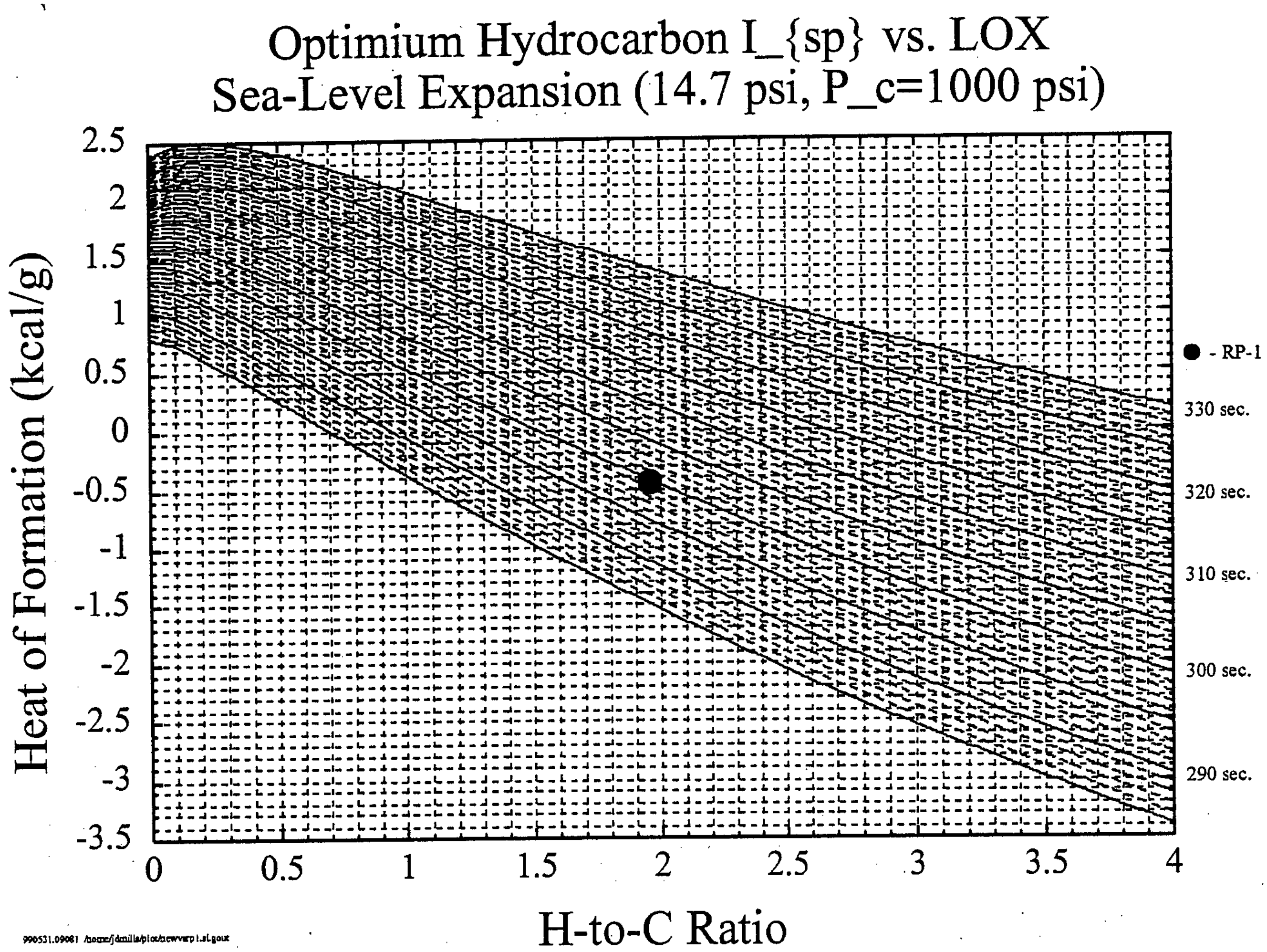
ρ_{of}–oxidizer-fuel bulk density

ρ_f–fuel density

a–density exponent (often, mission-specific constant)

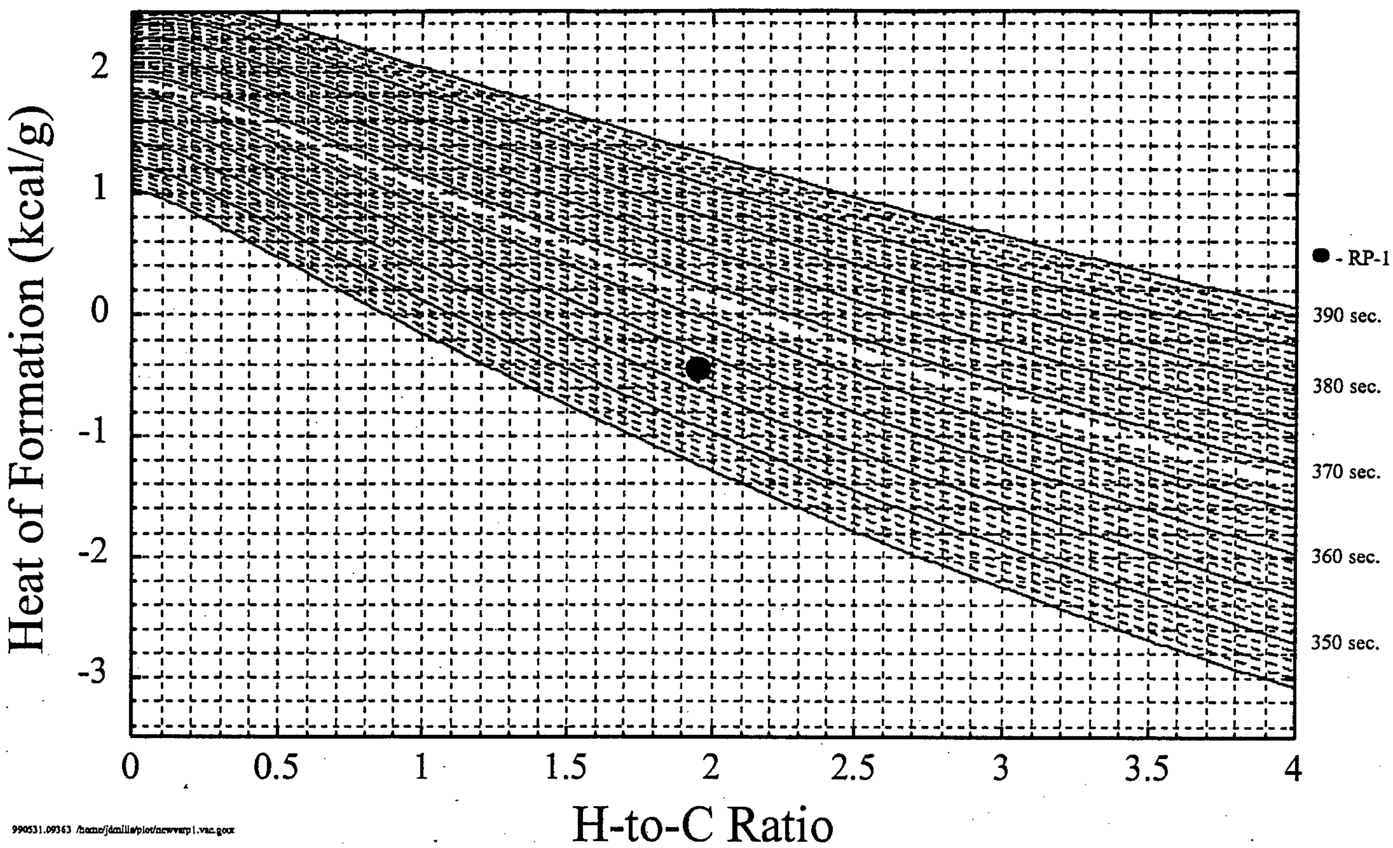
Optimium Hydrocarbon I_{sp} vs. LOX
Sea-Level Expansion (14.7 psi, P_c=1000 psi)





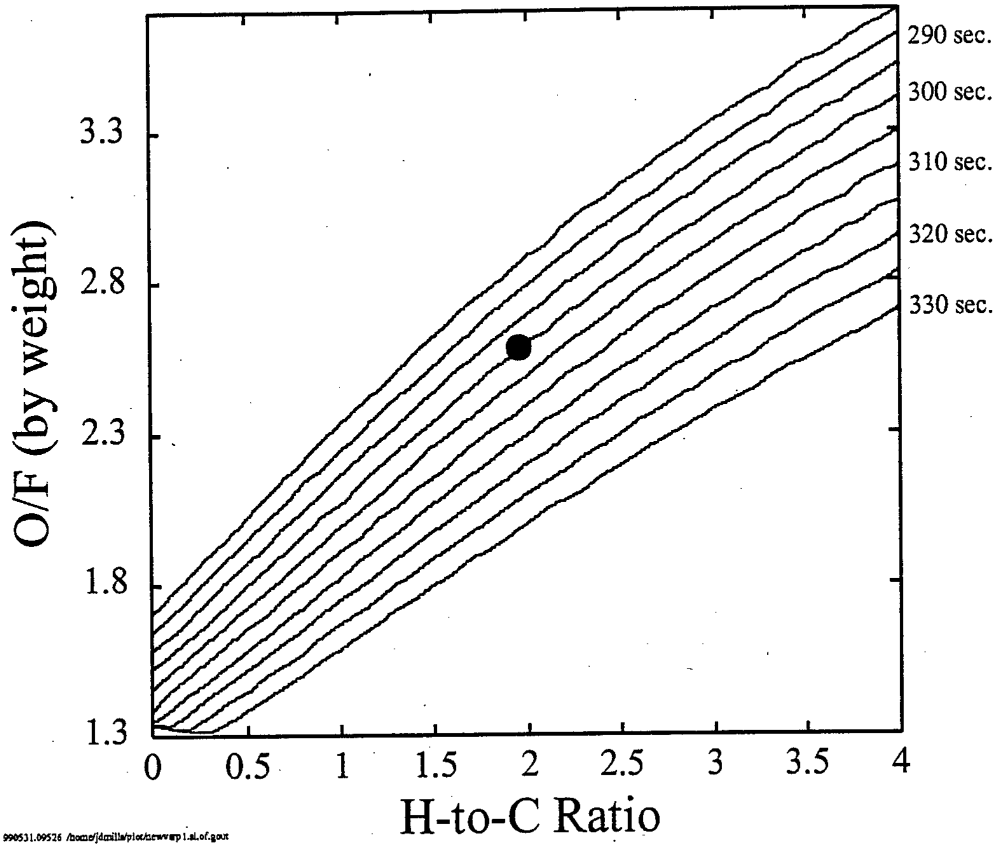
Optimium Hydrocarbon I_{sp} vs. LOX
Sea-Level Expansion (14.7 psi, P_c=1000 psi)
Heat of Formation (kcal/g)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
0
0.5
1
1.5
2
2.5
3
3.5
4
H-to-C Ratio
- RP-1
330 sec.
320 sec.
310 sec.
300 sec.
290 sec.
990531.09081

Optimium Hydrocarbon I_{sp} vs. LOX
Vacuum Expansion ({/Symbol e}=40, P_c=1000 psi)



990531.09363 /home/jdmills/plot/newvrp1.vac.gox

O/F at Optimium I_{sp}
Sea-Level Expansion (14.7 psi, P_c=1000 psi)



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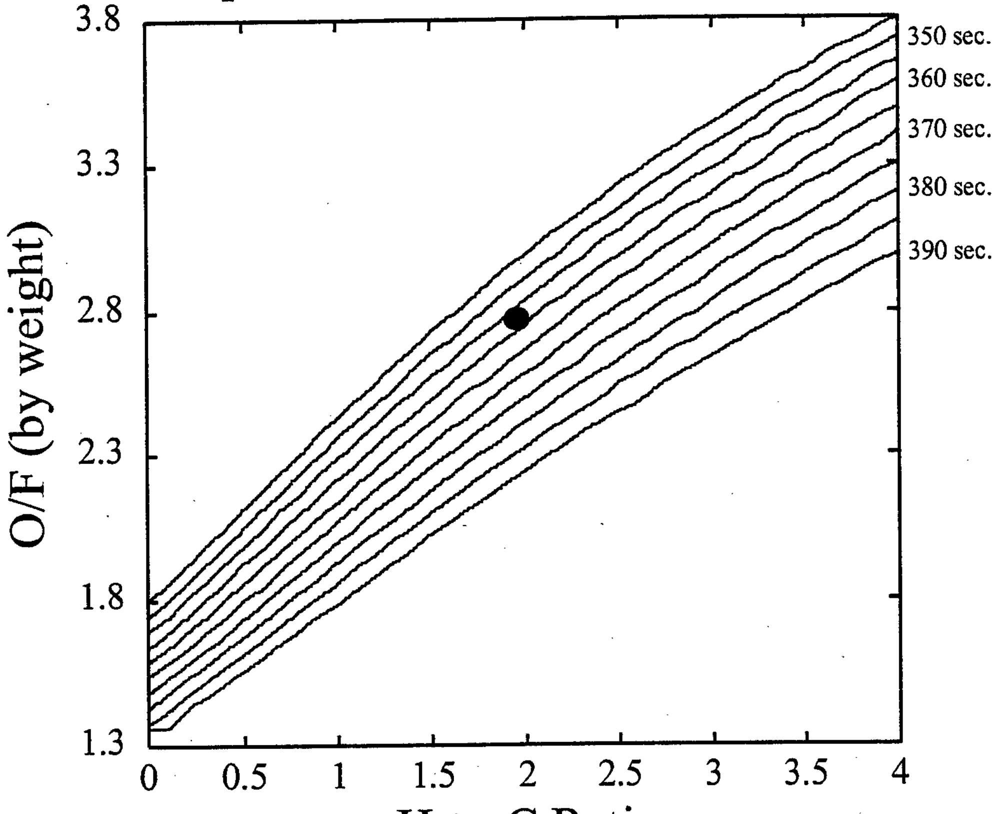
O/F at Optimium I_{sp}
Vacuum Expansion ({/Symbol e}=40, P_c=1000 psi)



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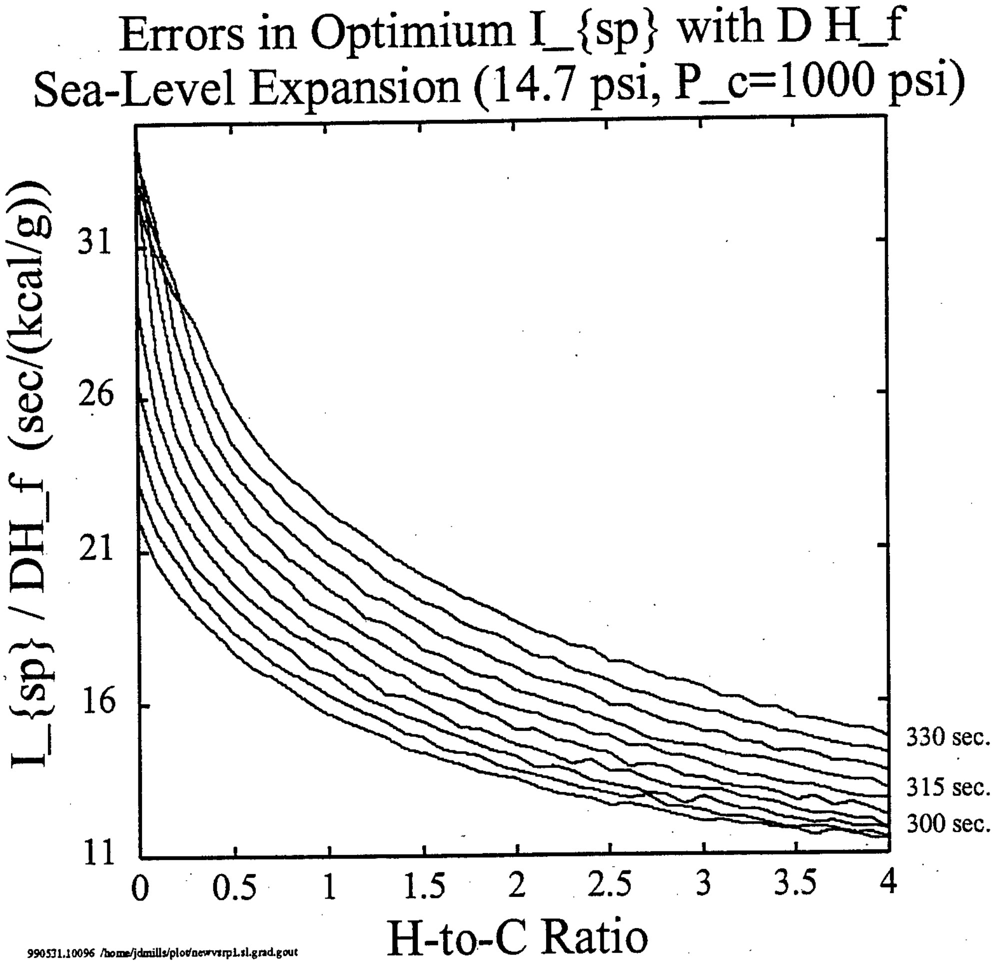
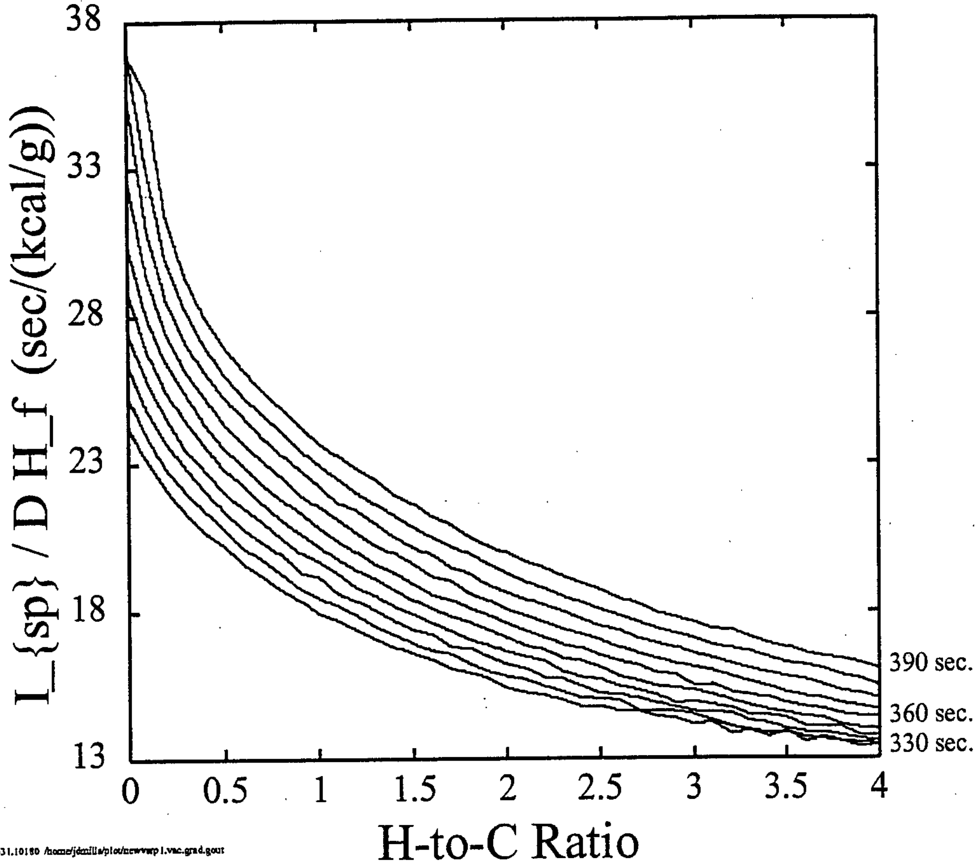


Errors in Optimium I_{sp} with D H_f
Sea-Level Expansion (14.7 psi, P_c=1000 psi)
I_{sp} / DH_f (sec/(kcal/g))
31
26
21
16
11
0
0.5
1
1.5
2
2.5
3
3.5
4
H-to-C Ratio
330 sec.
315 sec.
300 sec.
990531.10096 /home/jdmills/plot/newvsrp1.sl.grad.gout

Errors in Optimium I_{sp} with D H_f
Vacuum Expansion (e=40, P_c=1000 psi)



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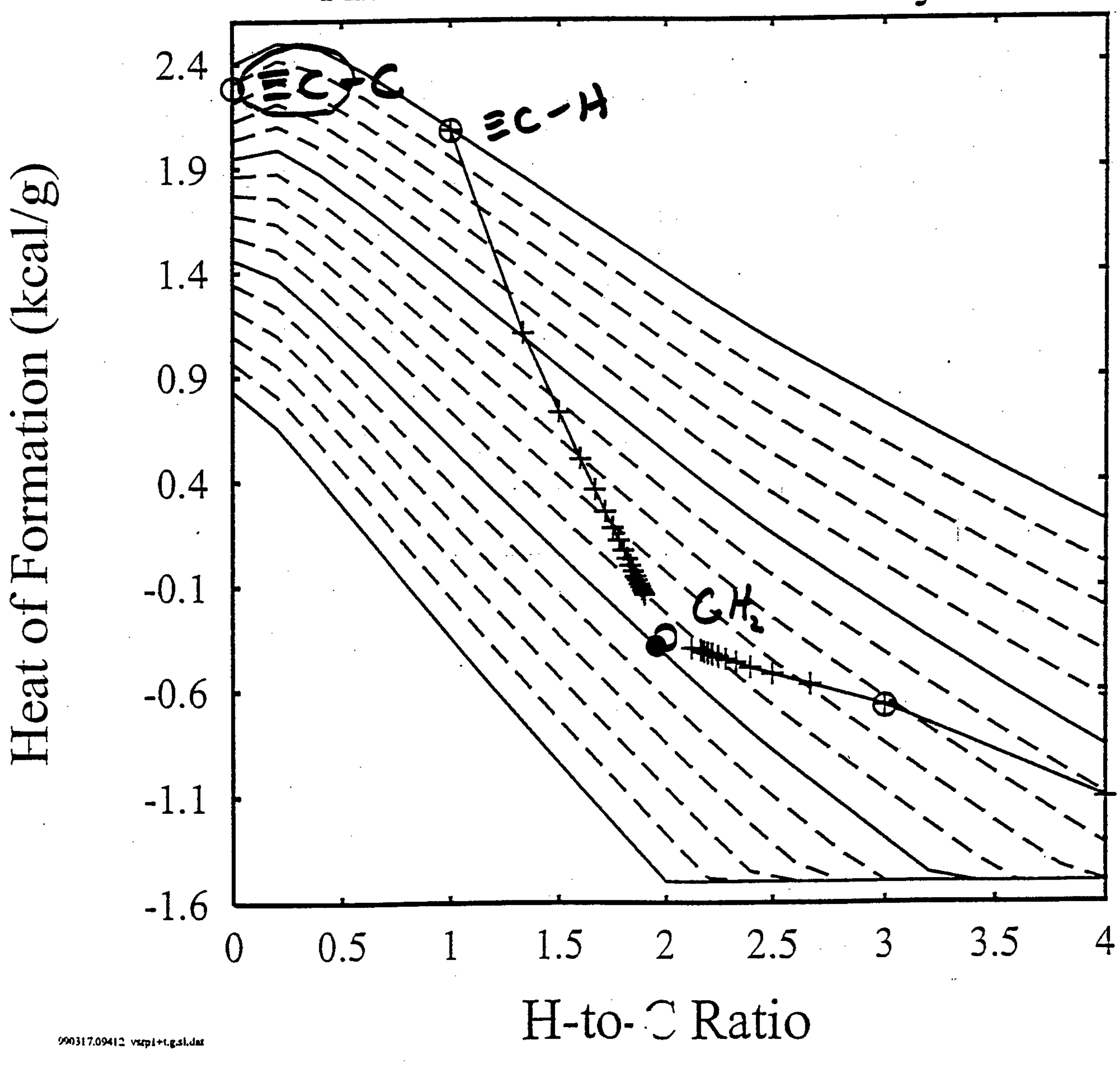
A Specific-Impulse Survey of Chemical Families—

Gas, Sea-Level Hydrocarbon Performance
Alkanes and Terminal Alkynes



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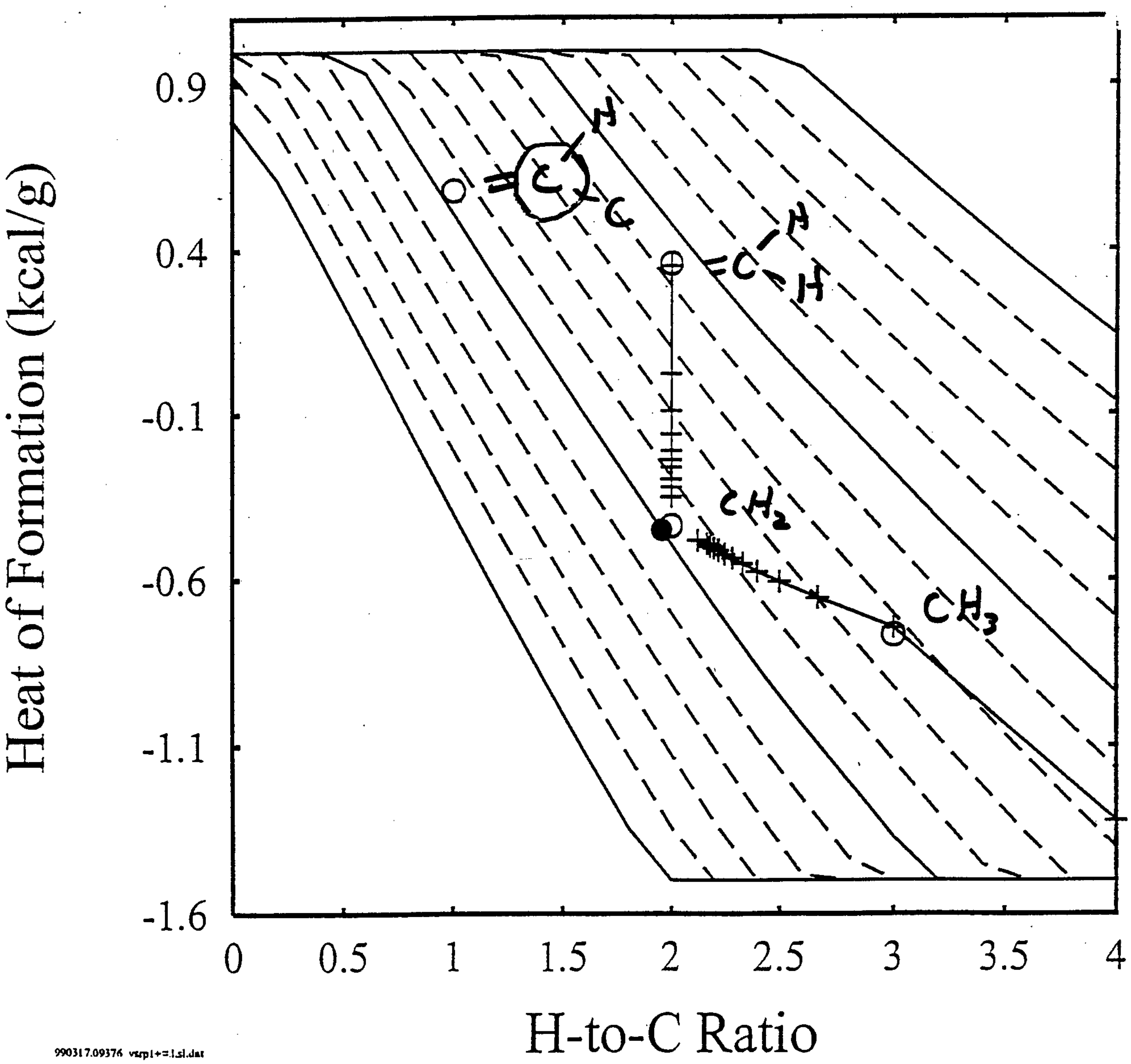
Liquid, Sea-Level Hydrocarbon Performance
Alkanes and Terminal Alkenes



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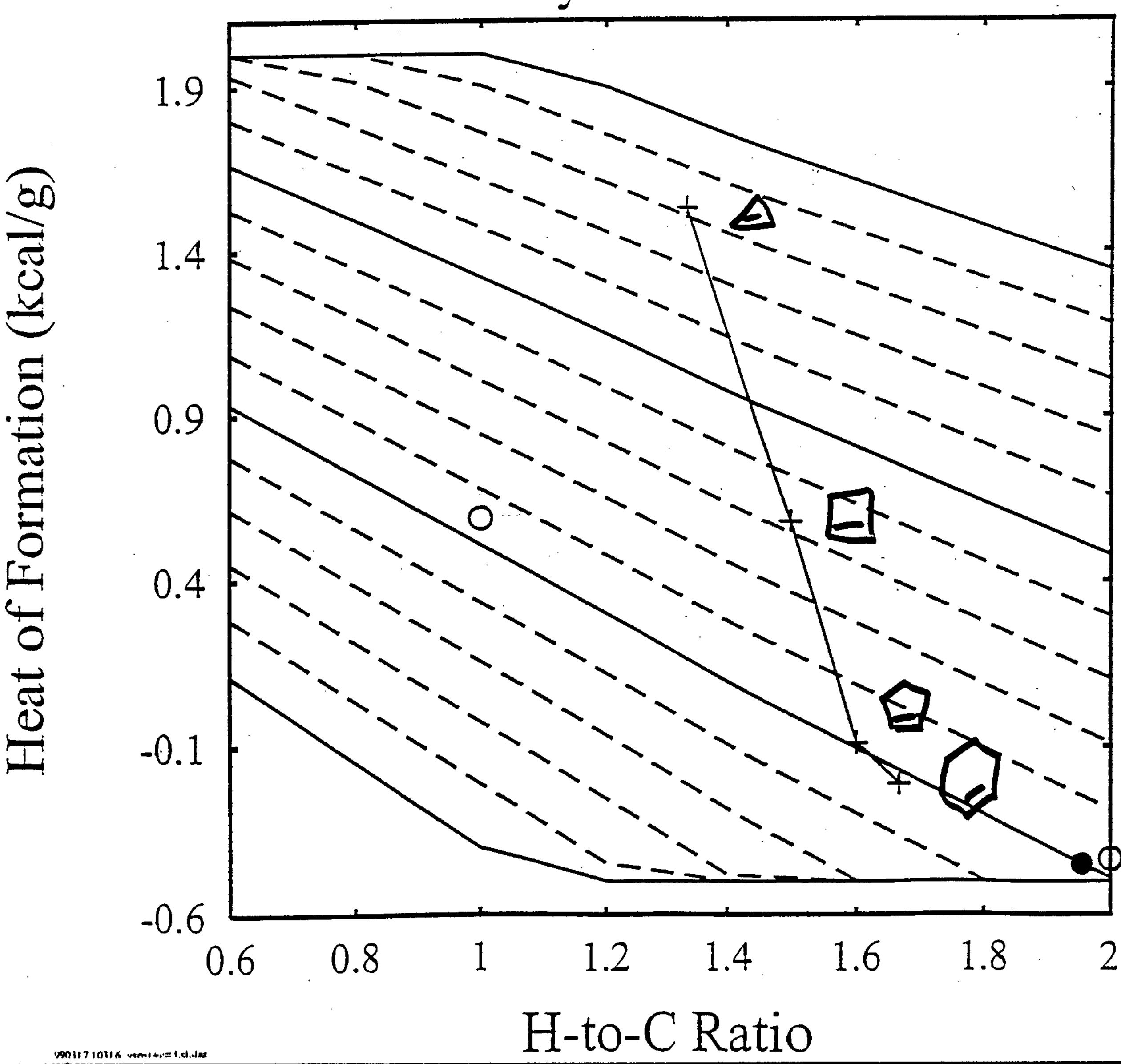
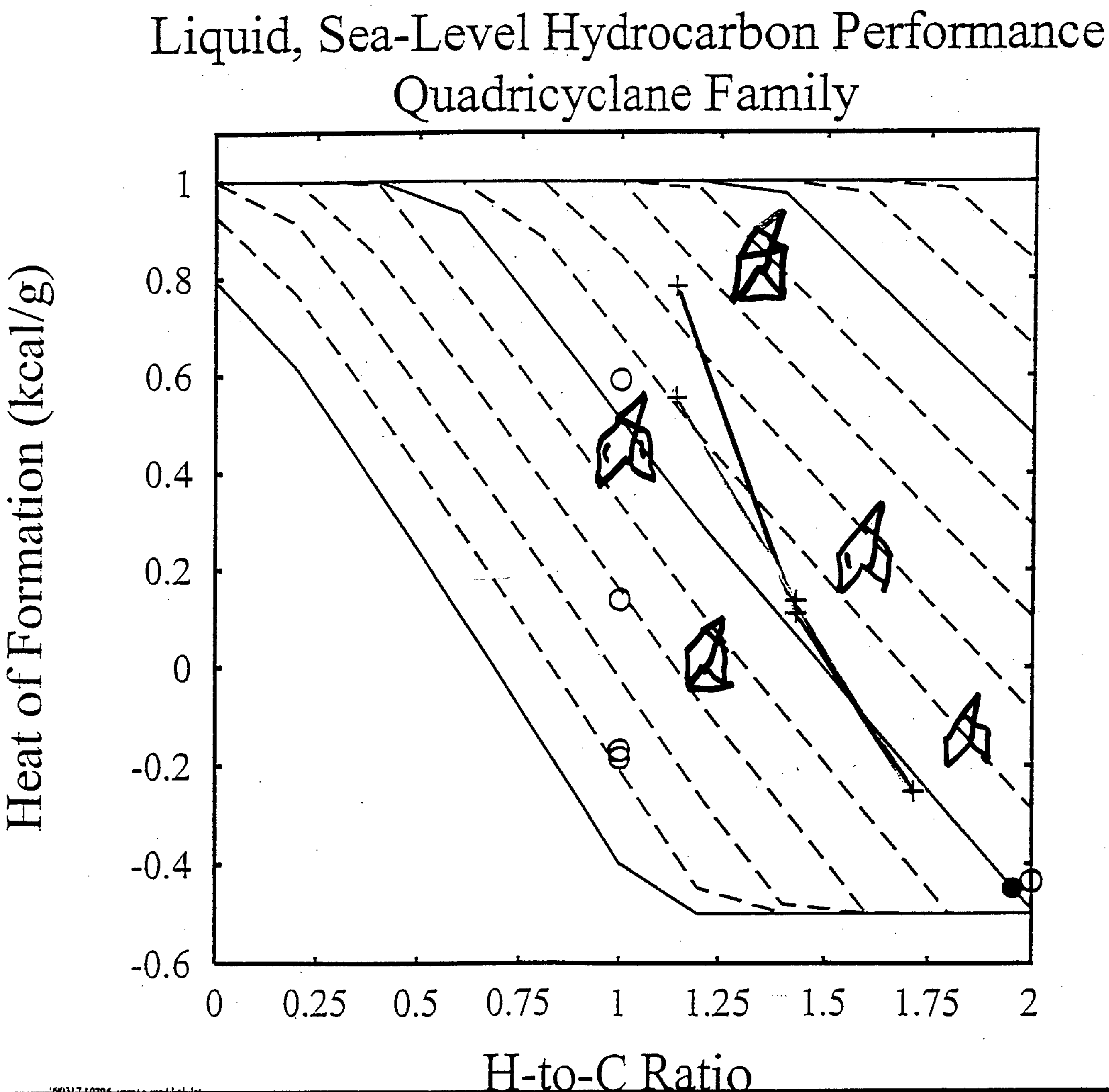
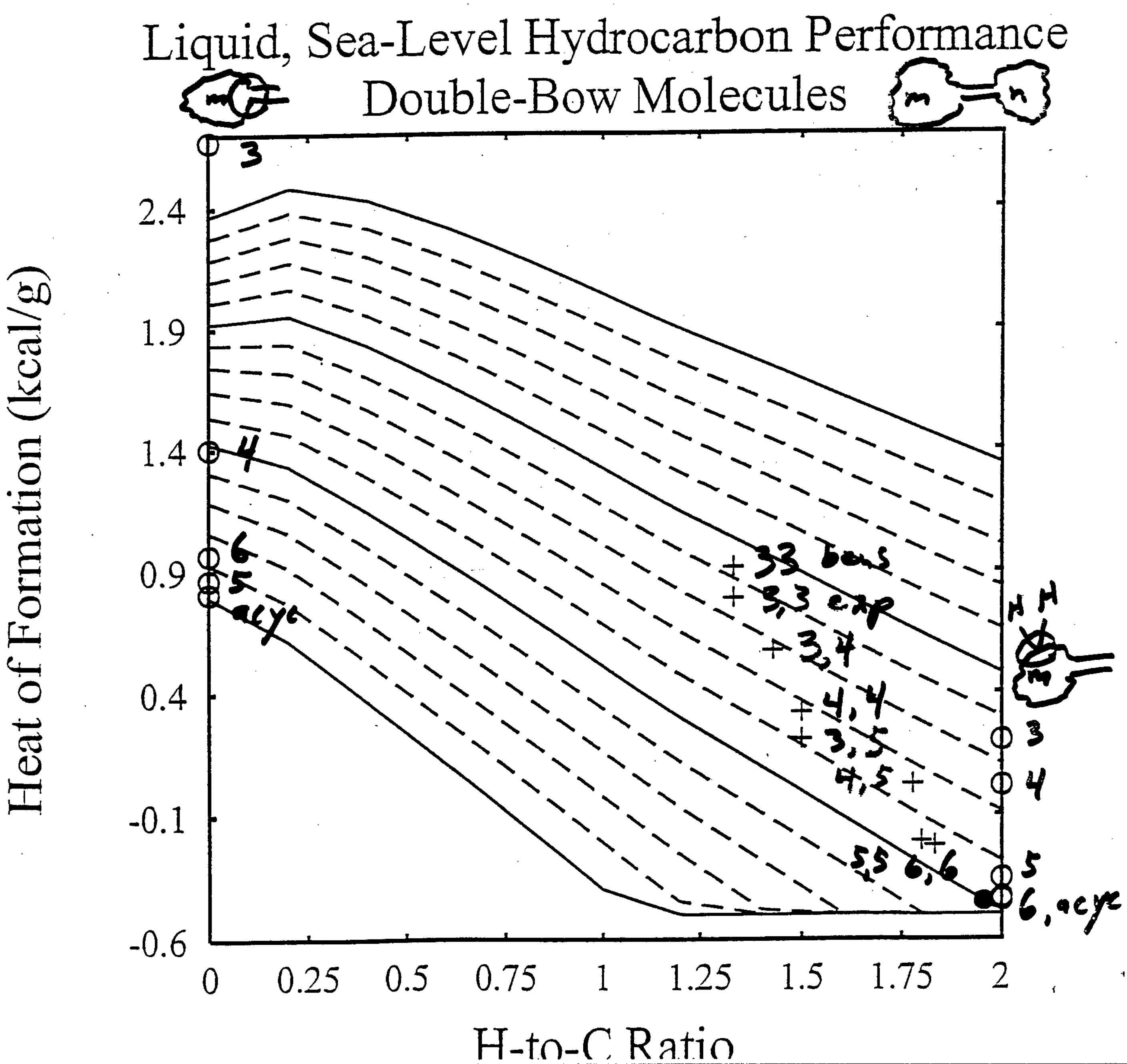
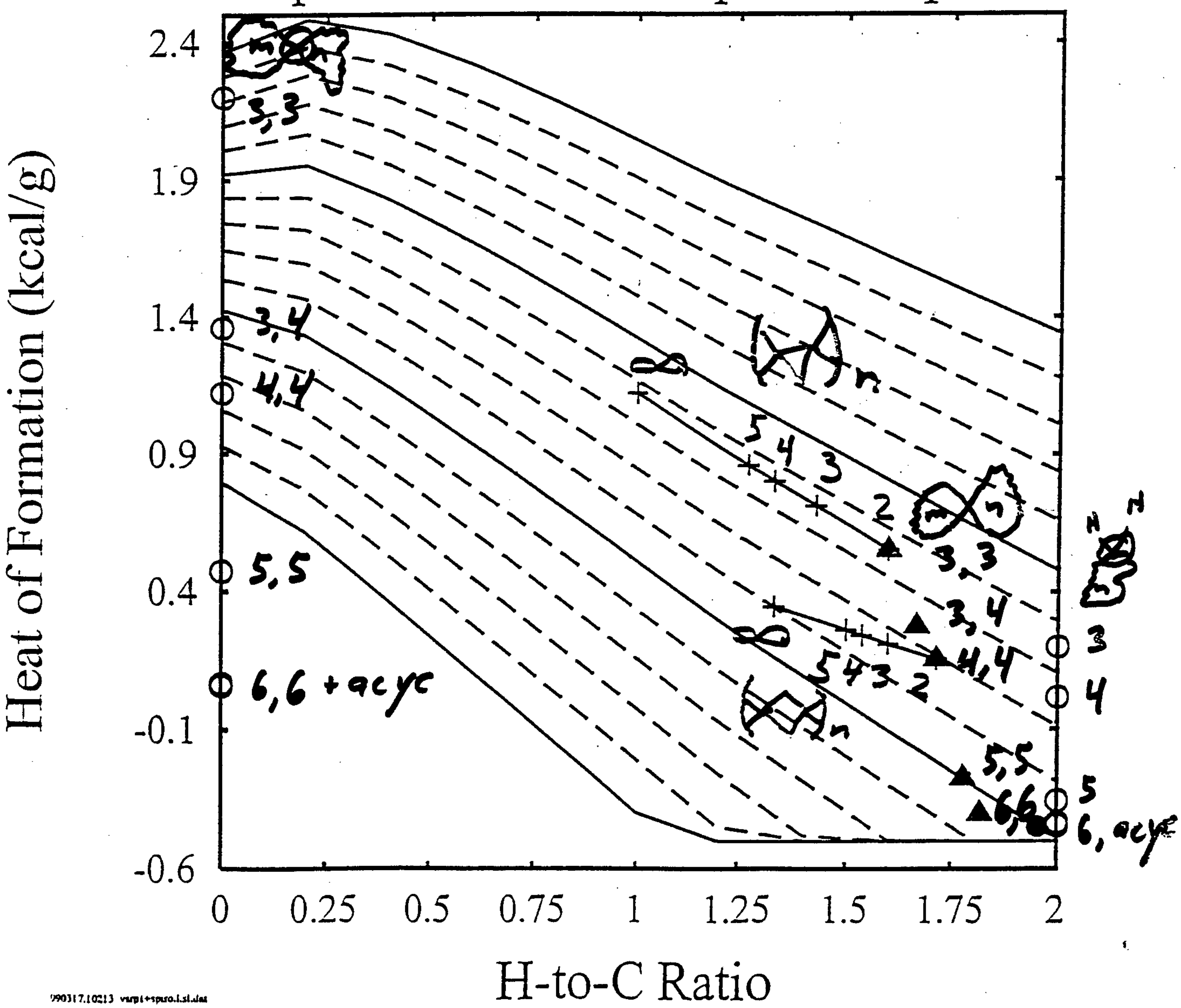
Liquid, Sea-Level Hydrocarbon Performance
Cycloalkenes




Liquid, Sea-Level Hydrocarbon Performance
Quadricyclane Family
Heat of Formation (kcal/g)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
0.25
0.5
0.75
1
1.25
1.5
1.75
2
H-to-C Ratio

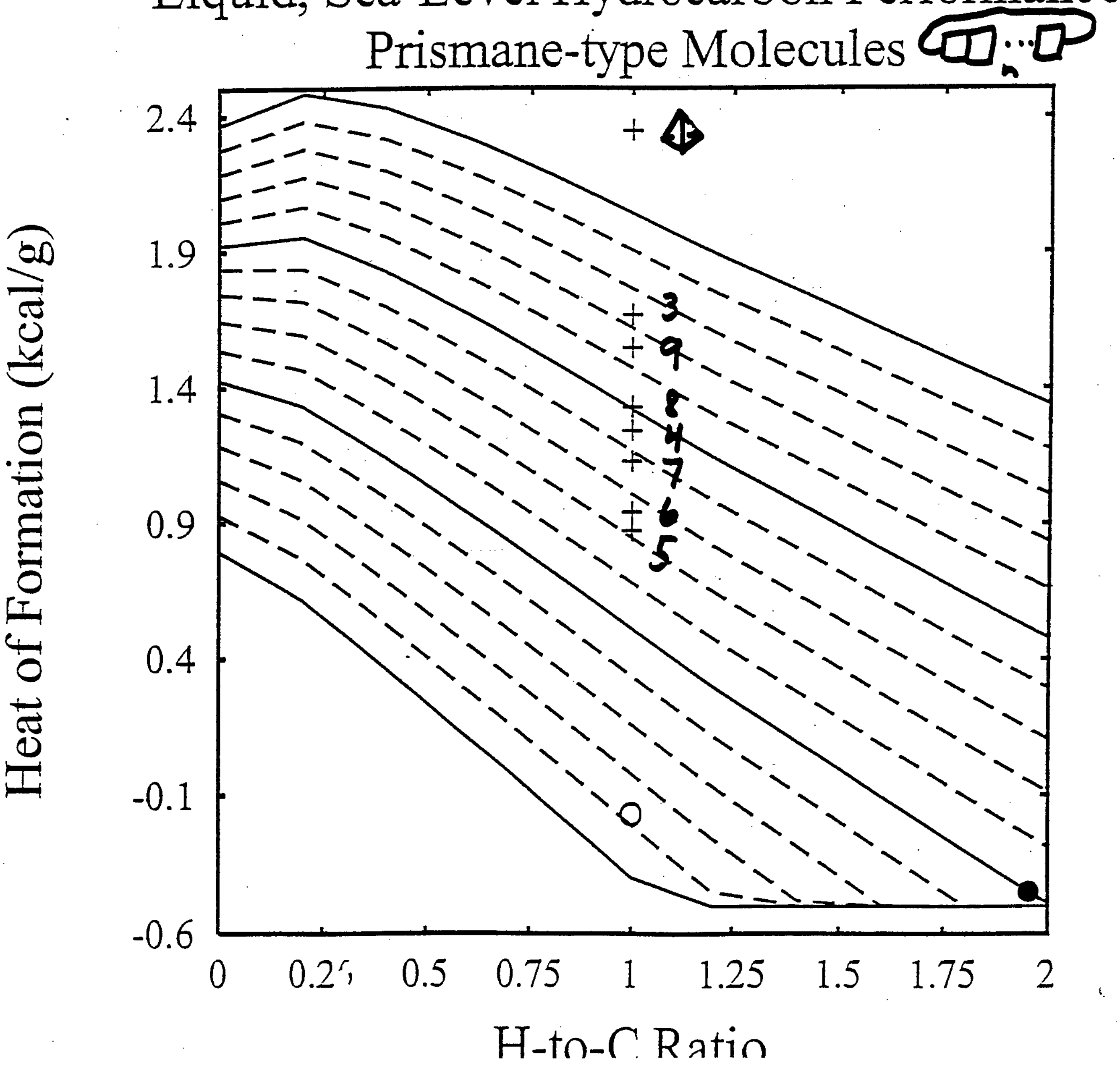

Liquid, Sea-Level Hydrocarbon Performance
Double-Bow Molecules
m
m
n
Heat of Formation (kcal/g)
2.4
1.9
1.4
0.9
0.4
-0.1
-0.6
0
0.25
0.5
0.75
1
1.25
1.5
1.75
2
H-to-C Ratio
3
4
6
5
acyc
3,3 bows
3,3 exp
3,4
4,4
3,5
4,5
5,5
6,6
H
H
3
4
5
6, acyc.

Liquid, Sea-Level Hydrocarbon Performance
Simple and Catenated Spiro Compounds



990317.10213 vapi+spiro.l.sl.dat

Liquid, Sea-Level Hydrocarbon Performance
Prismane-type Molecules



“Benson-Group” Specific Impulse–

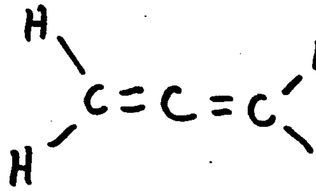
Additional Approximation: Benson-Group *Gedanken* Rocket

$$(I_{sp})_{opt} \approx \sum_{\substack{i \\ \text{groups}}} \frac{m_i}{m_{tot}} (I_{sp,i})_{opt}$$

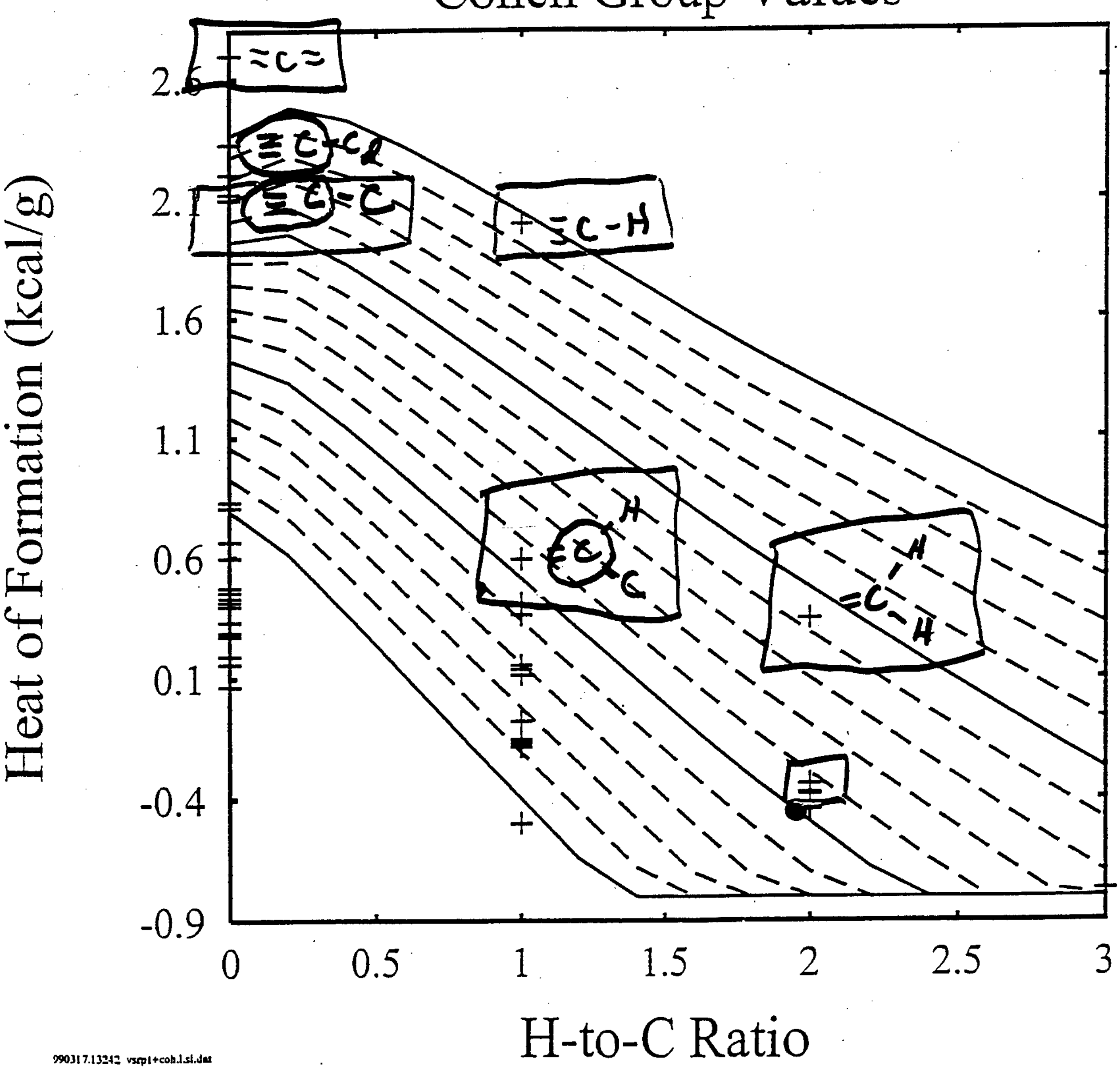
$\frac{m_i}{m_{tot}}$–group mass fraction

$(I_{sp,i})_{opt}$–optimized specific impulse for the chemical group, alone

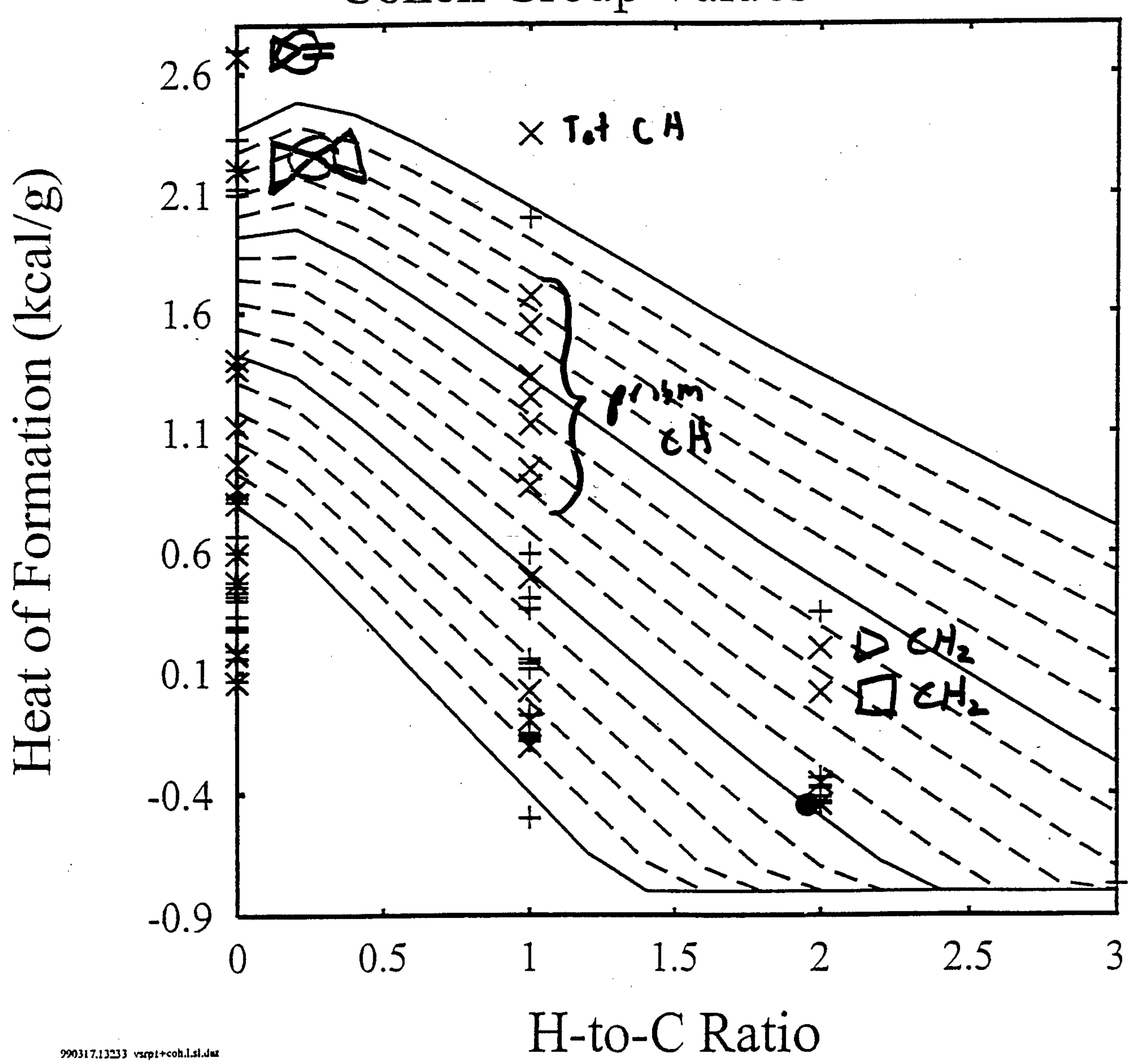
$H-C\equiv C-CH_2-$



Liquid, Sea-Level Hydrocarbon Performance
Cohen Group Values



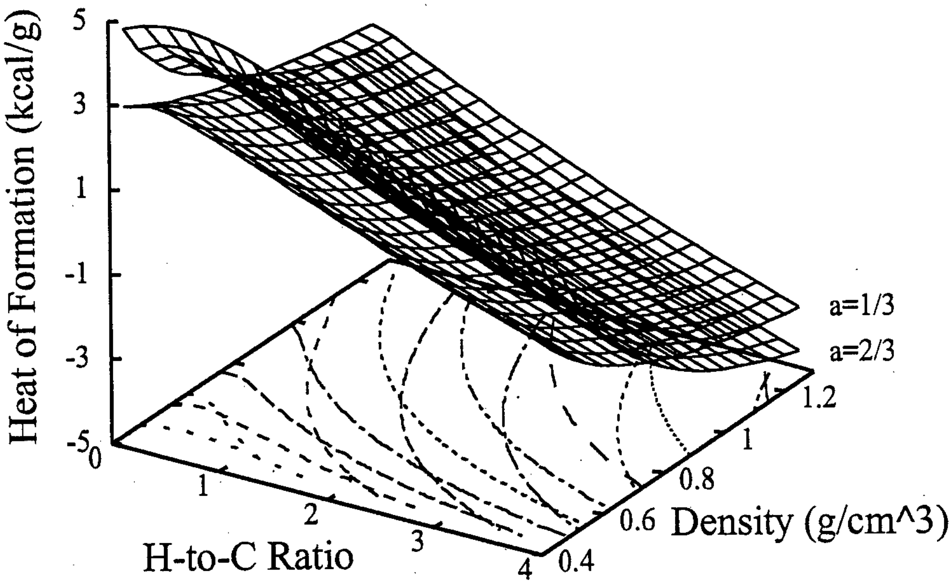
Liquid, Sea-Level Hydrocarbon Performance
Cohen Group Values + Extras



990317.13233 vsrpt+coh.l.sl.dat

Effects of Fuel Density–

Optimium Density I_{sp} vs. LOX
Sea-Level Expansion



Summary and Future Directions–

- Specific ΔH_f, $r(\frac{H}{C})$, and fuel density, alone, determine model, LOX-optimized rocket performance of hydrocarbon fuels
- Performance trade-offs among these parameters have been quantified and illustrated for ready reference
- Hydrocarbon fuels can be sought among known molecules in the parameterized performance space herein described
- The "Benson specific impulse" provides at least a semi-quantitative guide in the search for new, unknown rocket fuels

- **Other chemical systems may be explored using these insights (C,H,N; doped H_2)**

Acknowledgments–

These calculations were performed on local IBM RISC workstations using a modified version of the Air-Force specific-impulse rocket code written by C. Selph, R. Hall, C. Beckman, R. Acree, T. Magee and others.